



## wwPDB EM Validation Summary Report ⓘ

Jan 1, 2025 – 08:19 AM EST

PDB ID : 8SEW  
EMDB ID : EMD-40431  
Title : Cryo-EM Structure of RyR1 + ADP (Local Refinement of TMD)  
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.  
Deposited on : 2023-04-10  
Resolution : 2.89 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

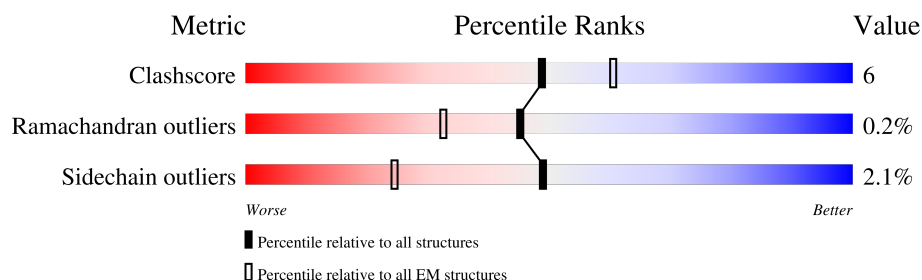
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	

## 2 Entry composition [i](#)

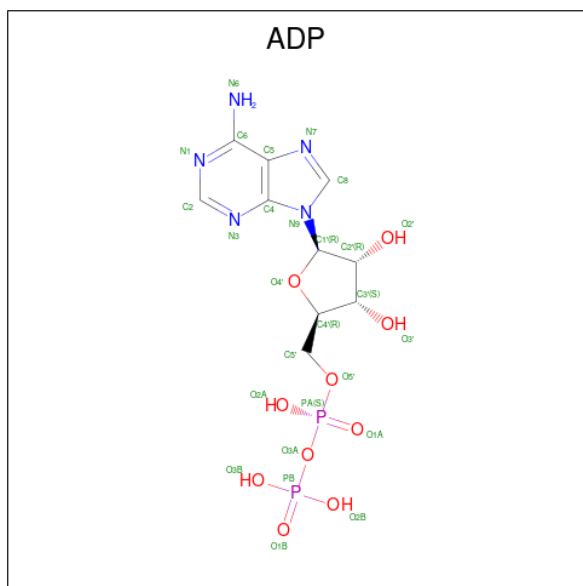
There are 3 unique types of molecules in this entry. The entry contains 20716 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	629	Total	C	N	O	S	0	0
			5151	3352	819	940	40		
1	B	629	Total	C	N	O	S	0	0
			5151	3352	819	940	40		
1	C	629	Total	C	N	O	S	0	0
			5151	3352	819	940	40		
1	D	629	Total	C	N	O	S	0	0
			5151	3352	819	940	40		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

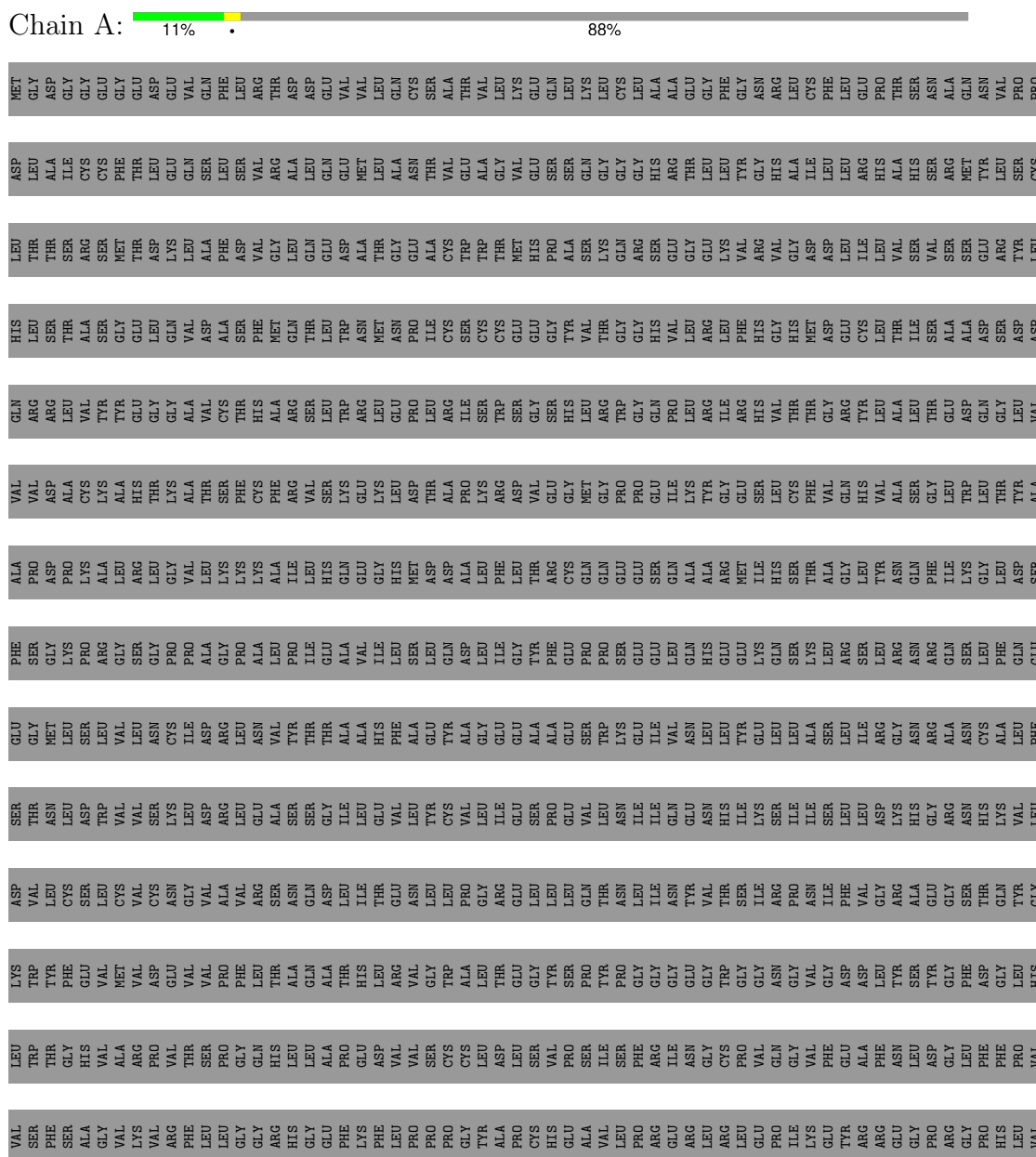
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ryanodine receptor 1



WORLDWIDE  
PDB  
PROTEIN DATA BANK

WORLDWIDE  
PDB  
PROTEIN DATA BANK







LEU	TRP	THR	GLY	TRP	THR	ASP	SER	GLU	PHE	ALA	VAL	GLN	HIS	LEU	ARG	GLN	HIS	LEU	THR	ASP	MET
TRP	THR	GLY	GLY	THR	ASP	LEU	ASN	GLY	SER	PRO	ASP	ARG	LEU	SER	GLY	THR	GLY	LEU	THR	LEU	GLY
GLY	HIS	GLU	SER	GLY	SER	SER	ASP	LEU	PRO	LYS	CYS	VAL	LEU	THR	VAL	LEU	THR	GLY	THR	ASP	GLY
VAL	VAL	VAL	LEU	ARG	TRP	LEU	TRP	GLY	ARG	ALA	LYS	TYR	SER	SER	TYR	TYR	GLY	SER	MET	CYS	GLY
ALA	ARG	MET	VAL	VAL	VAL	VAL	VAL	VAL	GLY	LEU	ALA	ALA	LEU	SER	GLY	GLY	GLY	GLY	PHE	GLY	GLY
ARG	PRO	ASP	GLY	SER	VAL	ASN	SER	ASN	SER	LEU	HIS	HIS	LEU	SER	GLY	GLY	HIS	GLY	THR	THR	GLY
PRO	ASP	CYS	GLY	GLY	LYS	CYS	LYS	GLY	PRO	GLY	LYS	GLY	LEU	GLY	THR	GLY	GLY	LEU	ASP	LEU	ASP
VAL	VAL	GLY	ASP	PRO	LEU	ILE	PRO	VAL	PRO	VAL	ALA	ALA	VAL	ARG	ALA	ALA	VAL	GLN	GLN	GLN	VAL
SER	VAL	VAL	ASP	ALA	ASP	ALA	GLY	ALA	GLY	LYS	SER	CYS	ALA	THR	THR	ASP	ALA	PHE	LEU	LEU	GLN
PRO	PRO	ALA	ARG	ARG	ARG	LEU	LEU	PRO	GLY	LYS	LEU	CYS	ALA	SER	THR	CYS	ALA	PHE	LEU	LEU	PHE
GLY	GLN	VAL	LEU	GLU	LEU	ASN	GLU	ASN	PRO	LYS	GLY	THR	SER	THR	THR	THR	PHE	ASP	SER	SER	LEU
LEU	LEU	ALA	GLY	THR	GLY	THR	ILE	ALA	ILE	GLN	GLY	LEU	LEU	ARG	GLN	GLY	GLY	GLY	ALA	GLY	GLY
ALA	ALA	ASP	SER	THR	GLY	ASP	GLY	ALA	GLY	HIS	SER	LEU	LEU	SER	LEU	TRP	GLY	GLY	GLY	GLY	GLY
PRO	THR	ILE	ILE	ALA	ILE	ASP	ILE	ALA	ALA	GLN	GLY	LEU	GLY	LEU	TRP	TRP	GLY	GLY	GLY	GLY	GLY
ASP	GLY	ILE	GLY	HIS	GLY	ILE	GLY	ILE	VAL	GLY	LYS	LEU	LEU	ARG	GLY	ARG	ASN	ALA	MET	LEU	VAL
VAL	ARG	GLY	VAL	VAL	VAL	GLY	VAL	PHE	ILE	HIS	LEU	GLY	ASN	GLY	GLY	GLY	ASN	GLY	ALA	GLY	ALA
VAL	VAL	ASN	VAL	VAL	VAL	ASN	VAL	ALA	GLY	GLY	ASP	PRO	PRO	GLY	GLY	GLY	GLY	GLY	ASN	GLY	GLY
SER	GLN	ASP	SER	THR	THR	THR	GLY	THR	ILE	LEU	SER	LEU	GLY	LEU	LEU	LEU	GLY	GLY	THR	GLY	GLY
LEU	ALA	LEU	GLY	THR	GLY	THR	SER	THR	GLY	HIS	LEU	LEU	GLY	LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY
ALA	ALA	ASP	GLY	THR	GLY	THR	GLY	THR	GLY	GLY	ASP	LEU	GLY	LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY
PRO	THR	ILE	ILE	ALA	ILE	ASP	ILE	ALA	ALA	GLN	SER	LEU	LEU	TRP	TRP	TRP	GLY	PHE	GLY	GLY	GLY
ASP	HIS	ILE	GLY	HIS	GLY	ILE	GLY	ILE	VAL	GLY	LYS	LEU	LEU	ARG	ARG	ASN	ASN	VAL	VAL	LEU	VAL
GLY	ASP	THR	LEU	LEU	THR	THR	VAL	PHE	ILE	GLY	LEU	GLY	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ALA	SER	NET	ASP	PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
SER	VAL	GLY	VAL	VAL	VAL	LEU	LEU	GLY	THR	ASP	THR	LEU	LEU	LEU	GLY	GLY	GLY	GLY	THR	THR	THR
SER	GLY	LEU	LEU	GLY	THR	LEU	TYR	GLY	GLY	ASP	THR	LEU	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	THR
CYS	TRP	LEU	CYS	TRP	CYS	LEU	CYS	TYR	GLN	ASP	ALA	LEU	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY
CYS	ALA	GLY	VAL	ALA	VAL	GLY	VAL	ALA	ASP	ALA	PRO	LEU	LEU	LEU	GLY	GLY	GLY	GLY	VAL	VAL	







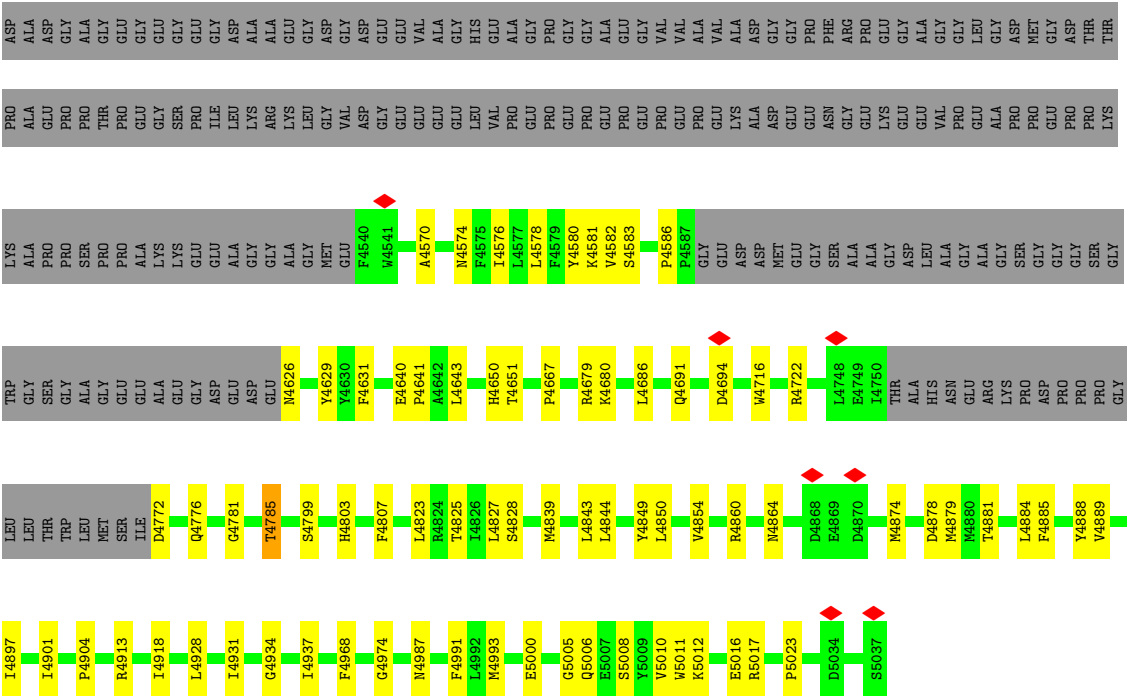




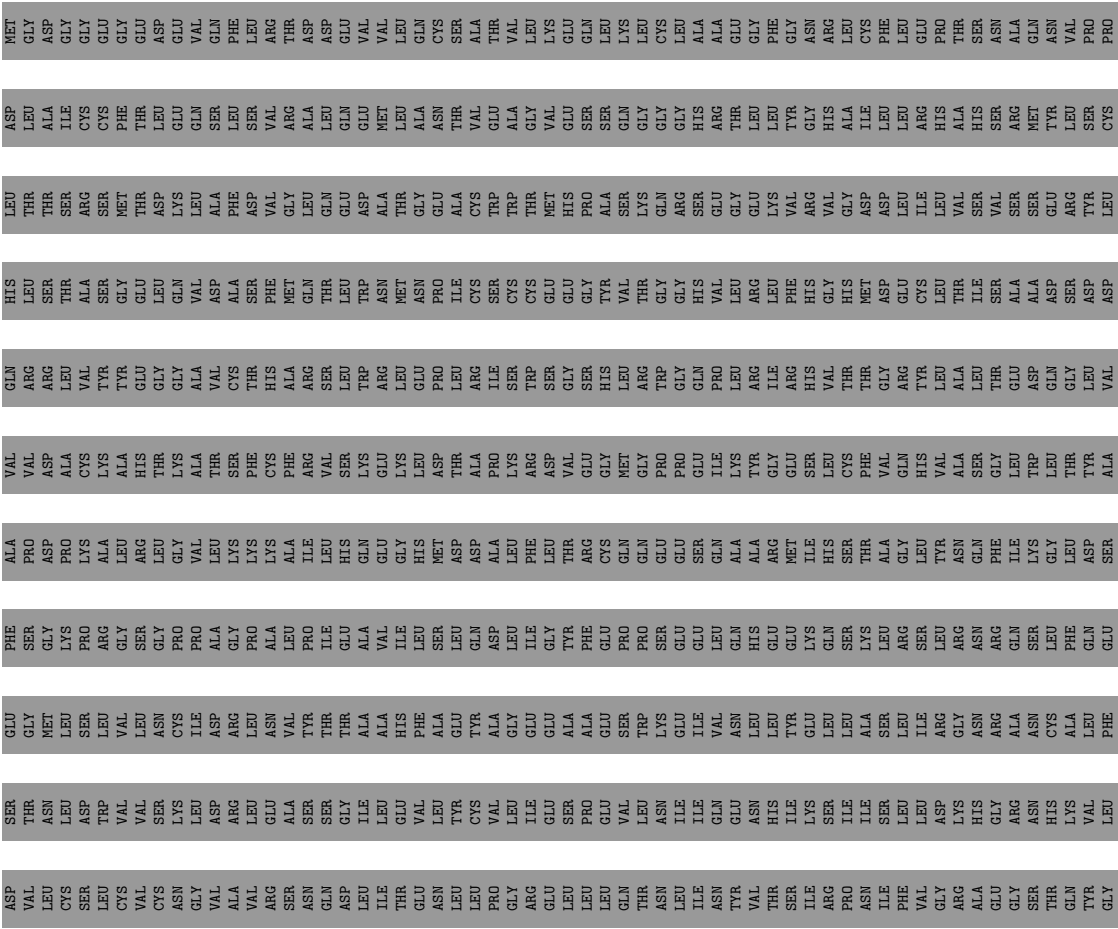








● Molecule 1: Ryanodine receptor 1









[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.054	Depositor
Minimum map value	-4.405	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.151	Depositor
Recommended contour level	0.483	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.28	0/5273	0.43	0/7116
1	B	0.28	0/5273	0.43	0/7116
1	C	0.28	0/5273	0.43	0/7116
1	D	0.28	0/5273	0.43	0/7116
All	All	0.28	0/21092	0.43	0/28464

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5151	0	5039	78	0
1	B	5151	0	5039	76	0
1	C	5151	0	5039	80	0
1	D	5151	0	5039	75	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	20716	0	20204	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 229 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4823:LEU:HG	1:B:4839:MET:CE	2.14	0.77
1:A:4839:MET:CE	1:D:4823:LEU:HG	2.14	0.77
1:C:4823:LEU:HG	1:D:4839:MET:CE	2.14	0.77
1:B:4823:LEU:HG	1:C:4839:MET:CE	2.14	0.77
1:B:4823:LEU:HG	1:C:4839:MET:HE2	1.73	0.70

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	619/5037 (12%)	605 (98%)	13 (2%)	1 (0%)	44	73
1	B	619/5037 (12%)	605 (98%)	13 (2%)	1 (0%)	44	73
1	C	619/5037 (12%)	605 (98%)	13 (2%)	1 (0%)	44	73
1	D	619/5037 (12%)	605 (98%)	13 (2%)	1 (0%)	44	73
All	All	2476/20148 (12%)	2420 (98%)	52 (2%)	4 (0%)	45	73

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	4691	GLN
1	B	4691	GLN
1	C	4691	GLN
1	D	4691	GLN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	561/4276 (13%)	549 (98%)	12 (2%)	48	78
1	B	561/4276 (13%)	549 (98%)	12 (2%)	48	78
1	C	561/4276 (13%)	549 (98%)	12 (2%)	48	78
1	D	561/4276 (13%)	549 (98%)	12 (2%)	48	78
All	All	2244/17104 (13%)	2196 (98%)	48 (2%)	49	78

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4580	TYR
1	C	4884	LEU
1	C	4626	ASN
1	C	4722	ARG
1	D	3992	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ADP	D	5101	-	24,29,29	0.76	0	29,45,45	0.85	2 (6%)
2	ADP	A	5101	-	24,29,29	0.76	0	29,45,45	0.85	2 (6%)
2	ADP	C	5101	-	24,29,29	0.76	0	29,45,45	0.85	2 (6%)
2	ADP	B	5101	-	24,29,29	0.76	0	29,45,45	0.85	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	D	5101	-	-	4/12/32/32	0/3/3/3
2	ADP	A	5101	-	-	4/12/32/32	0/3/3/3
2	ADP	C	5101	-	-	4/12/32/32	0/3/3/3
2	ADP	B	5101	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5101	ADP	C4'-O4'-C1'	-2.25	107.87	109.92
2	B	5101	ADP	C4'-O4'-C1'	-2.25	107.87	109.92
2	C	5101	ADP	C4'-O4'-C1'	-2.25	107.87	109.92
2	D	5101	ADP	C4'-O4'-C1'	-2.25	107.87	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5101	ADP	C5-C6-N6	2.08	123.48	120.31

There are no chirality outliers.

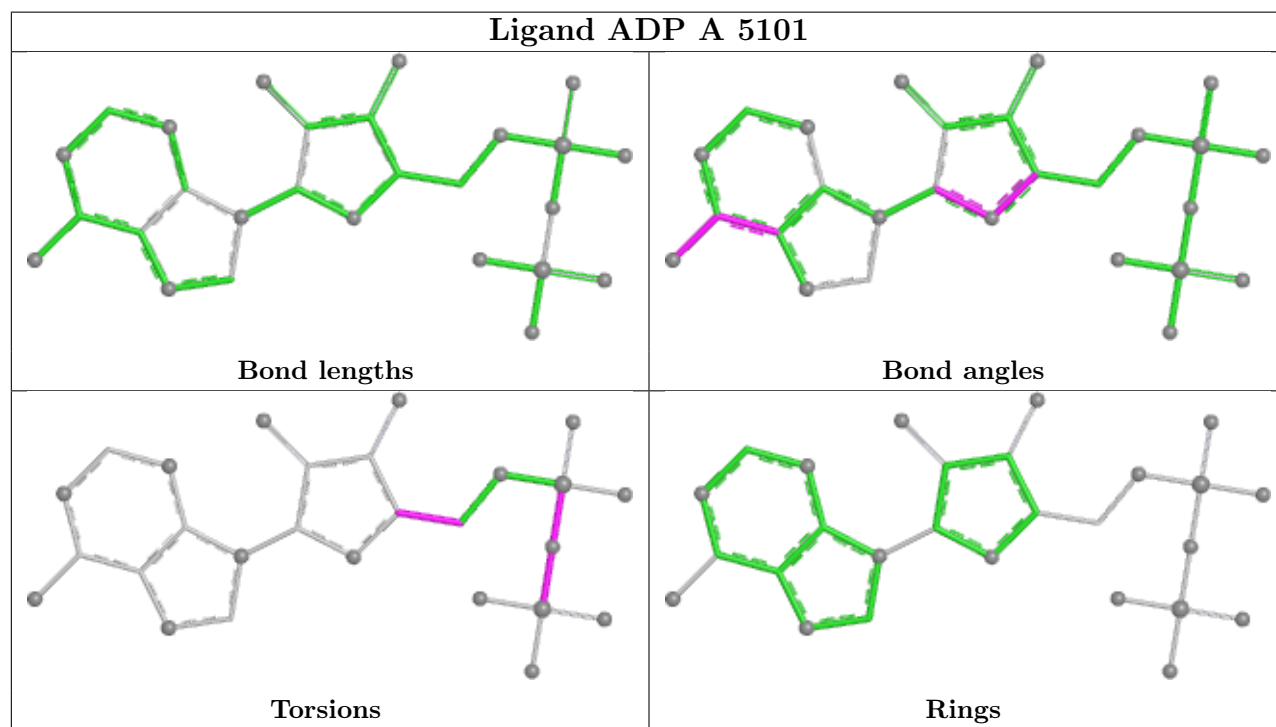
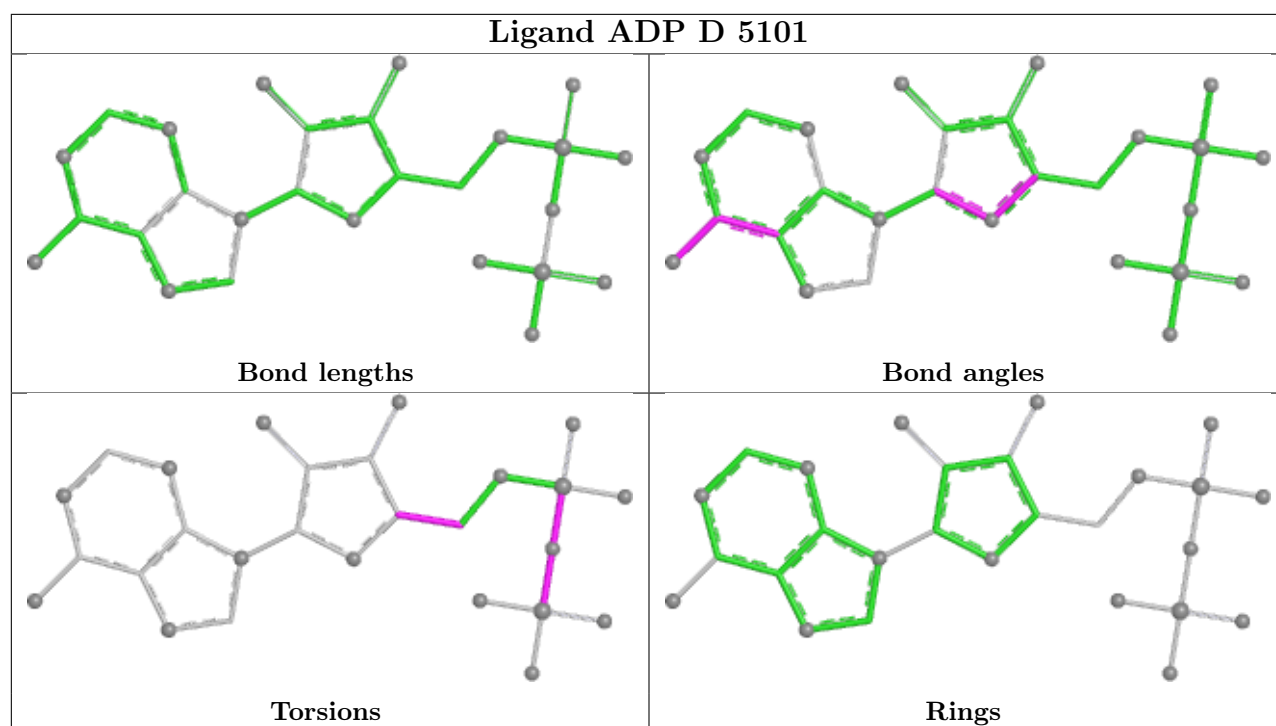
5 of 16 torsion outliers are listed below:

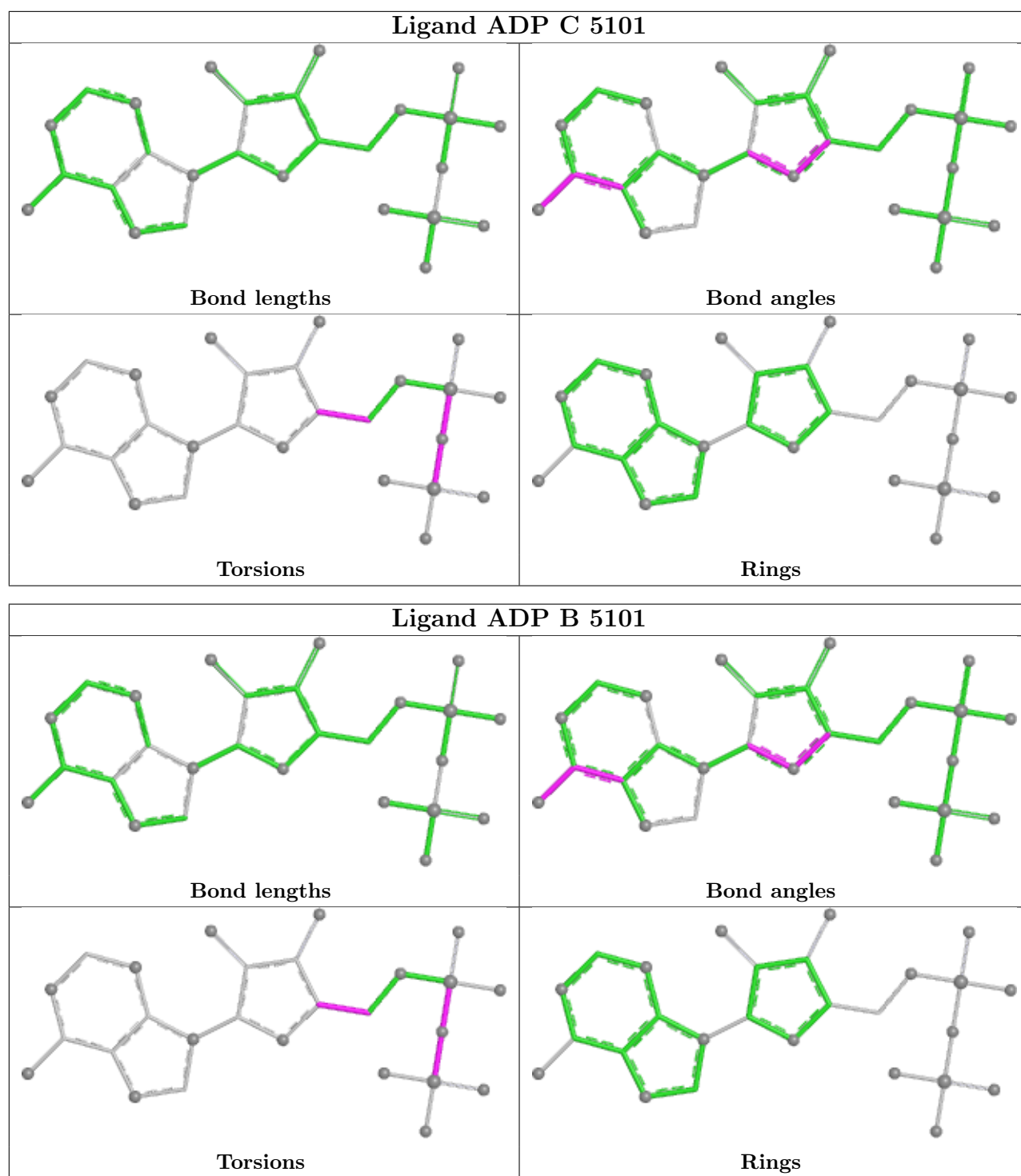
Mol	Chain	Res	Type	Atoms
2	A	5101	ADP	O4'-C4'-C5'-O5'
2	B	5101	ADP	O4'-C4'-C5'-O5'
2	C	5101	ADP	O4'-C4'-C5'-O5'
2	D	5101	ADP	O4'-C4'-C5'-O5'
2	A	5101	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

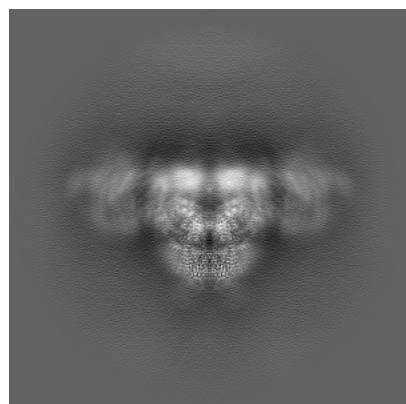
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40431. These allow visual inspection of the internal detail of the map and identification of artifacts.

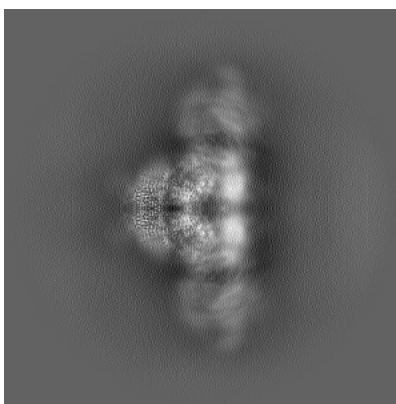
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

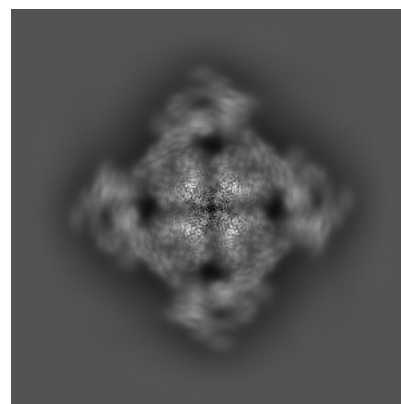
#### 6.1.1 Primary map



X

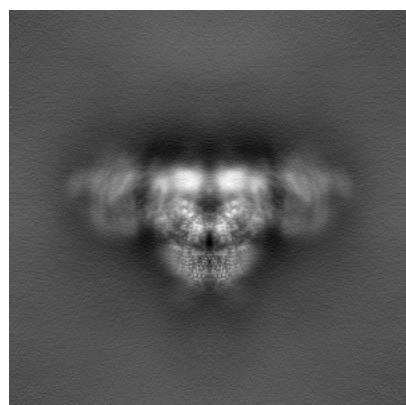


Y

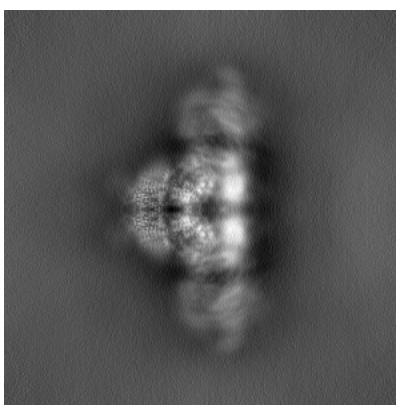


Z

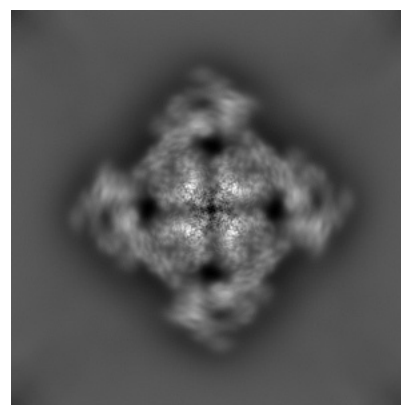
#### 6.1.2 Raw map



X



Y

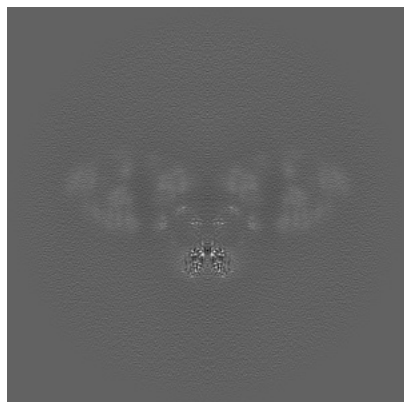


Z

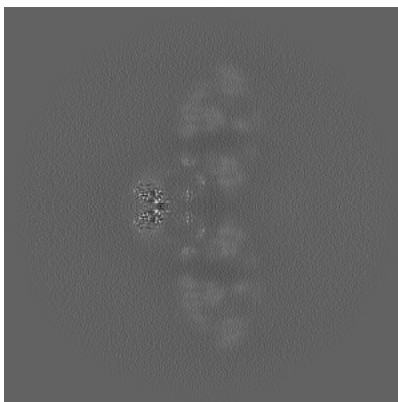
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

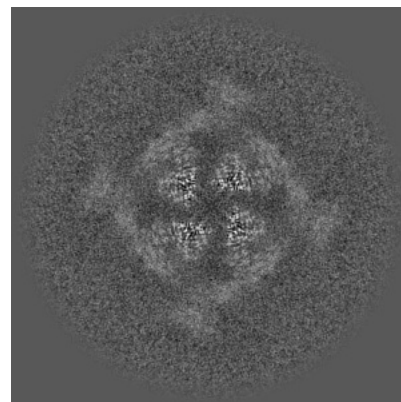
### 6.2.1 Primary map



X Index: 200

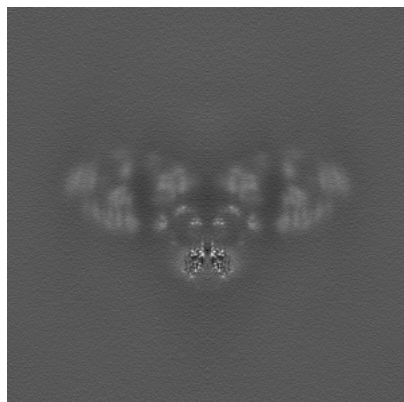


Y Index: 200

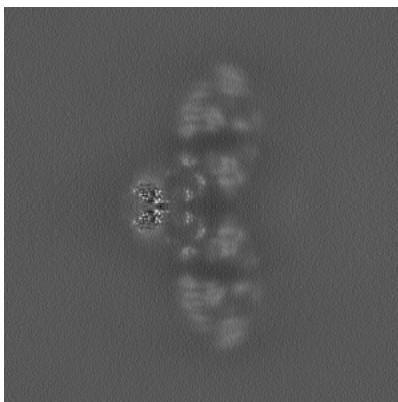


Z Index: 200

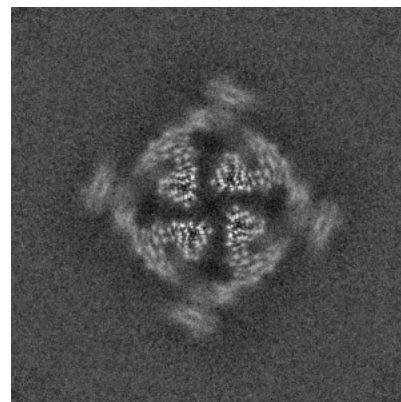
### 6.2.2 Raw map



X Index: 200



Y Index: 200



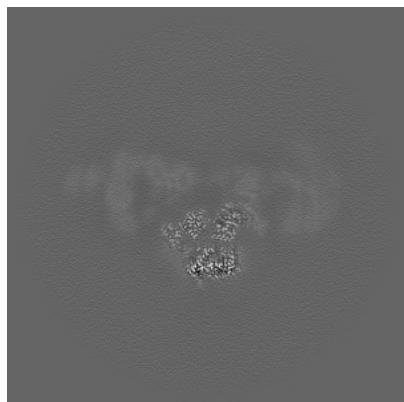
Z Index: 200

The images above show central slices of the map in three orthogonal directions.

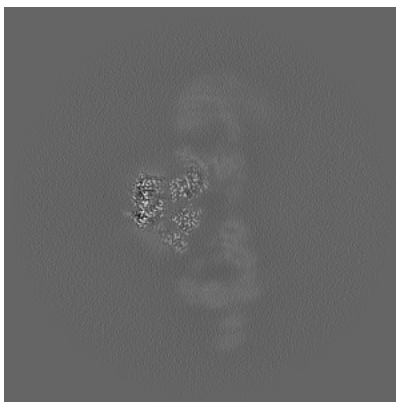


## 6.3 Largest variance slices [i](#)

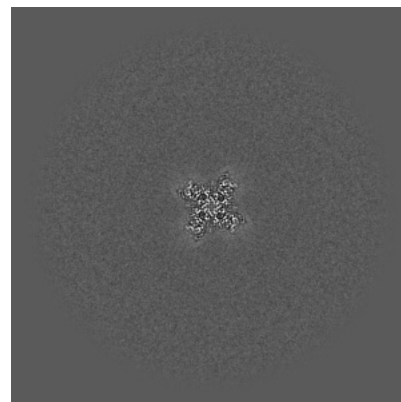
### 6.3.1 Primary map



X Index: 212

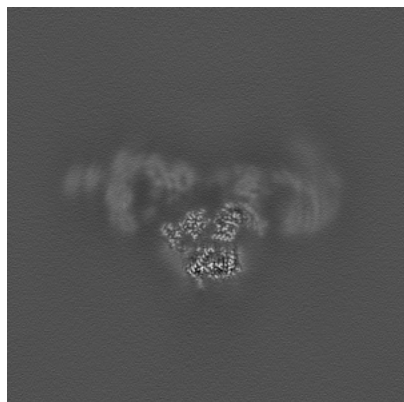


Y Index: 188

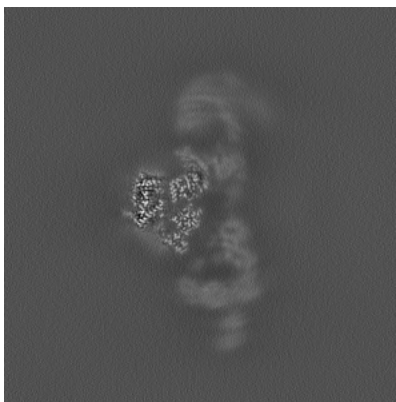


Z Index: 139

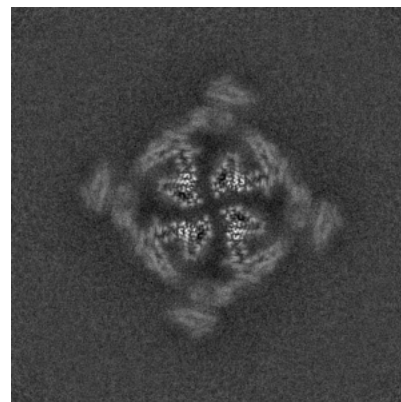
### 6.3.2 Raw map



X Index: 212



Y Index: 188

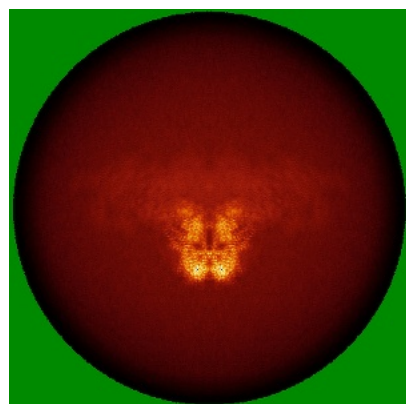


Z Index: 197

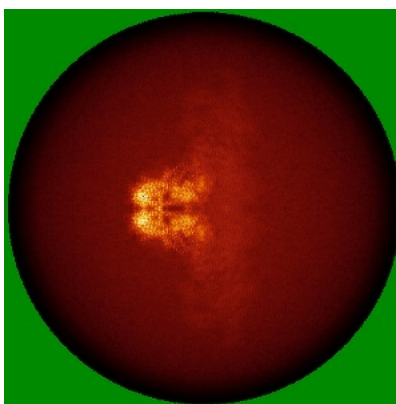
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

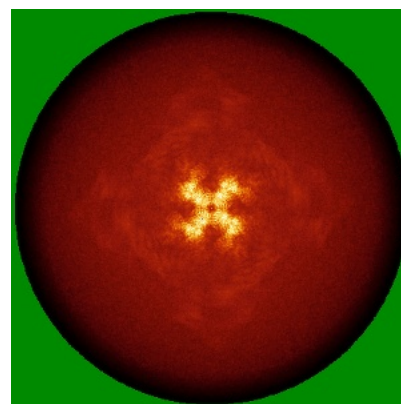
### 6.4.1 Primary map



X

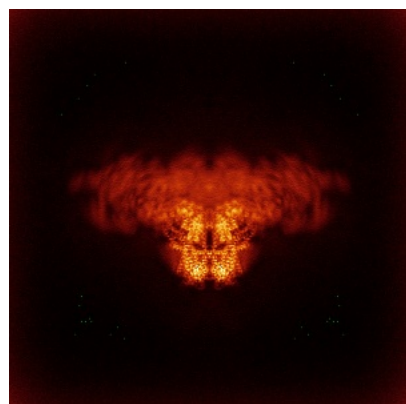


Y

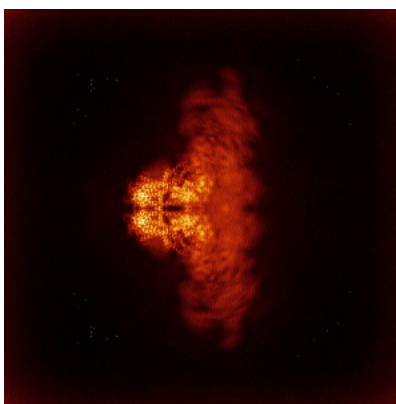


Z

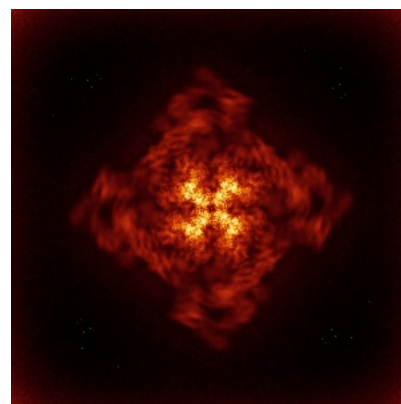
### 6.4.2 Raw map



X



Y

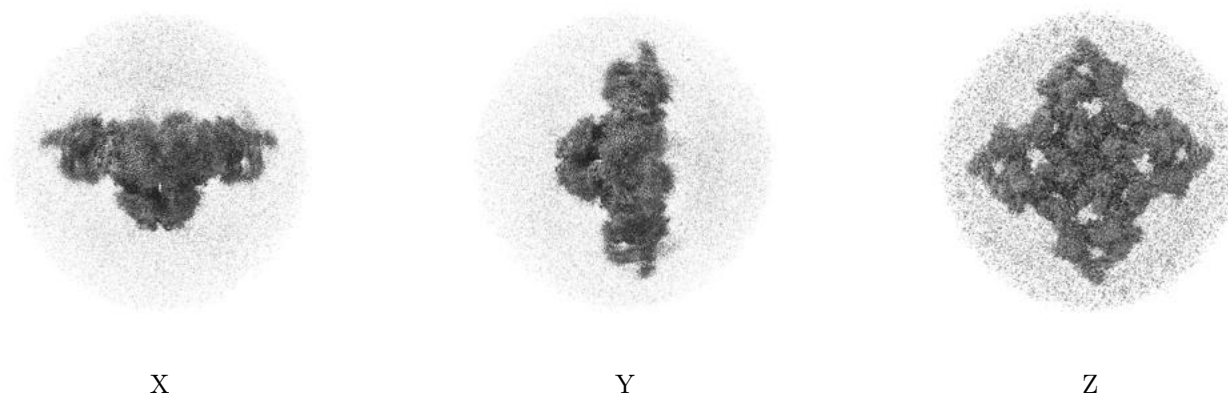


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.483. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

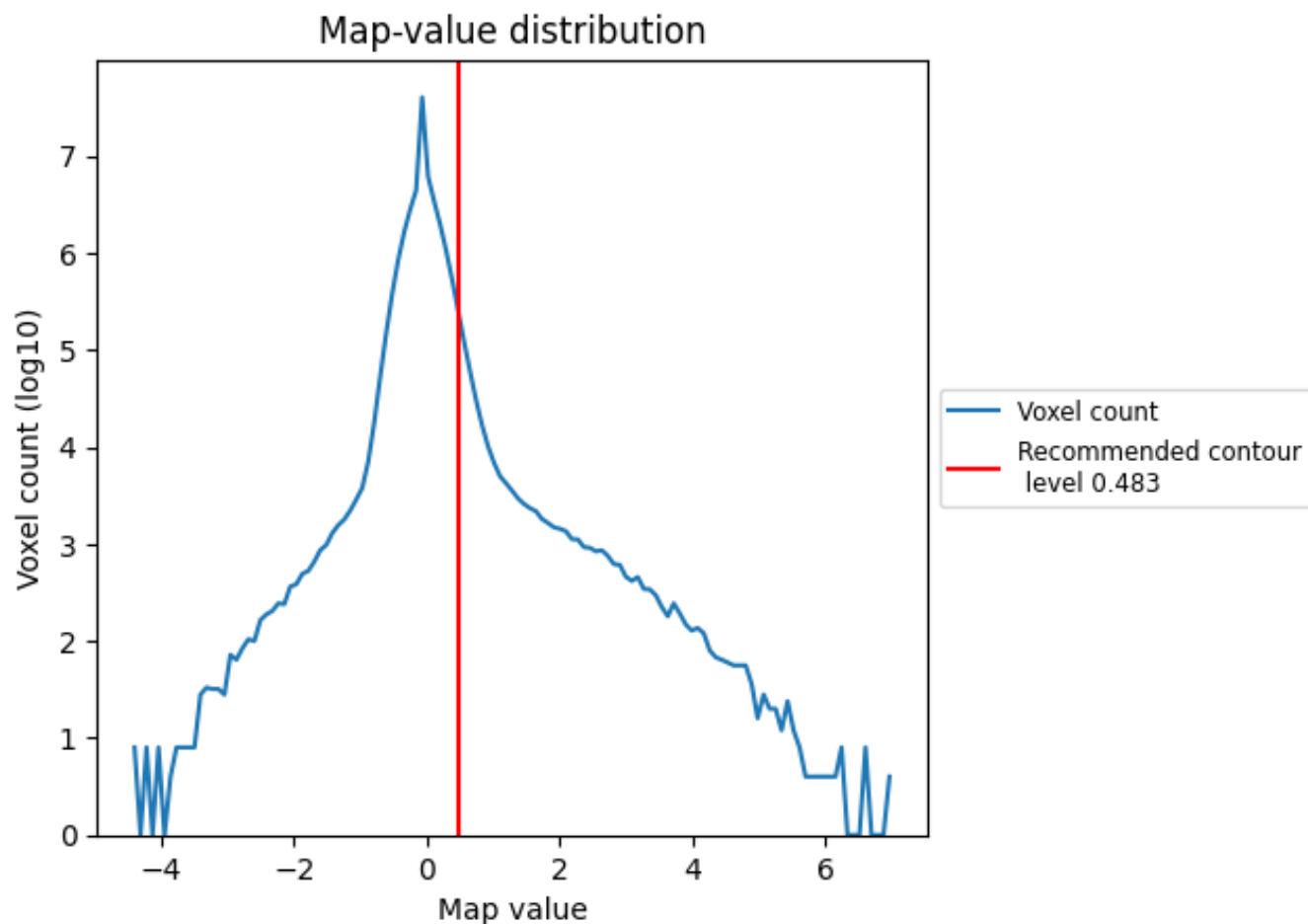
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

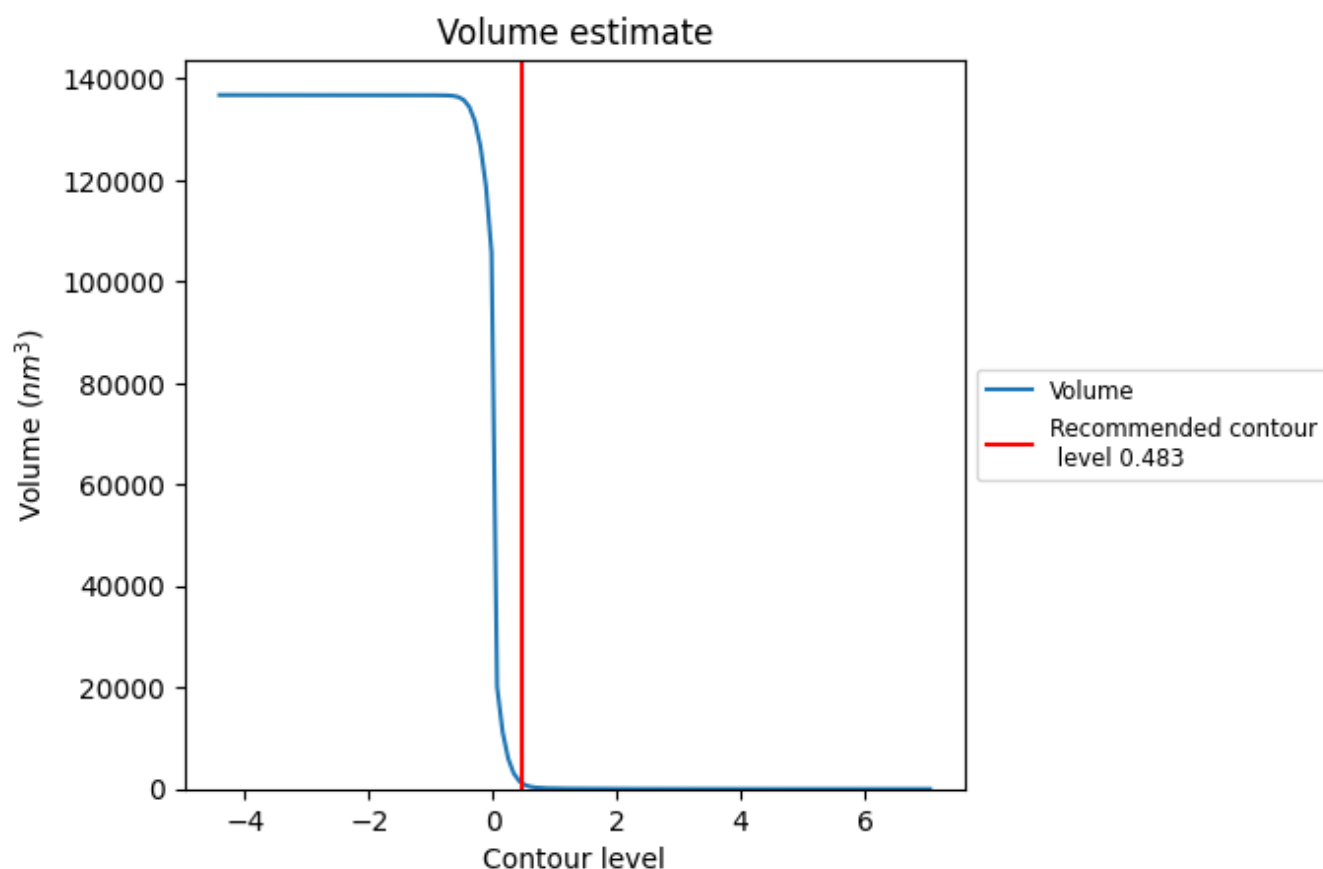
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

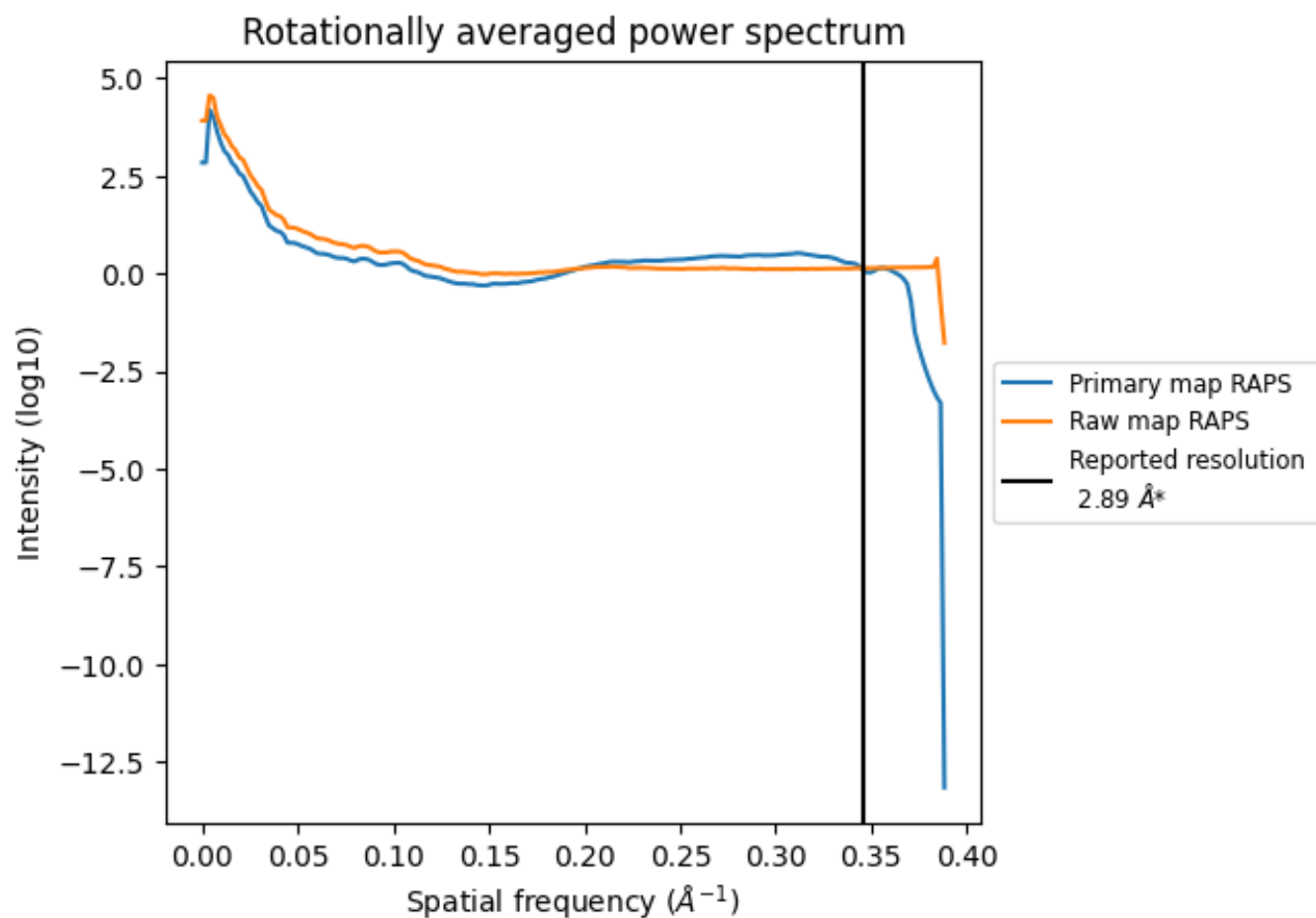
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1097  $\text{nm}^3$ ; this corresponds to an approximate mass of 991 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

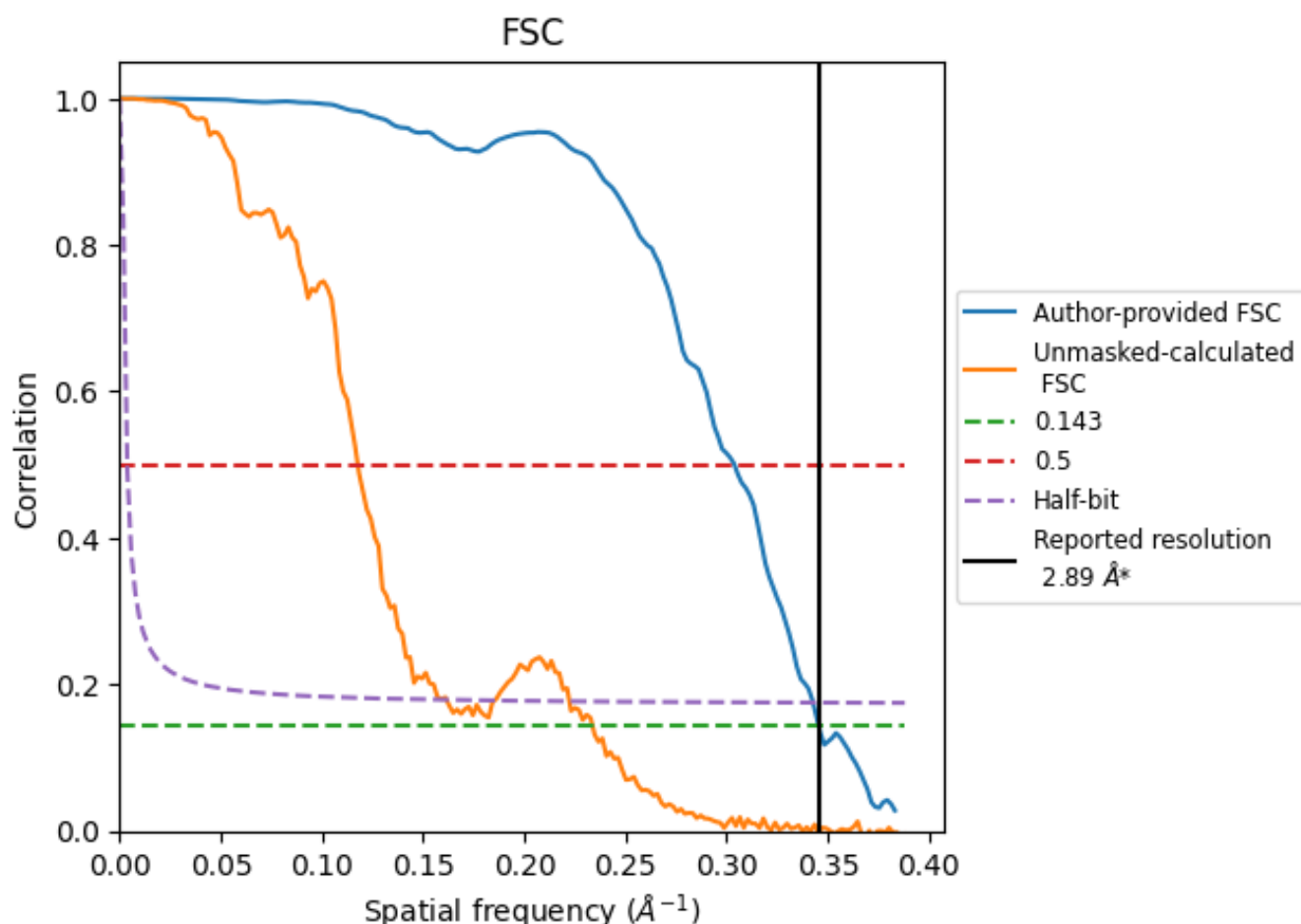


\*Reported resolution corresponds to spatial frequency of  $0.346 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.346  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.89	3.29	2.92
Unmasked-calculated*	4.28	8.49	6.18

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.28 differs from the reported value 2.89 by more than 10 %



## 9 Map-model fit [i](#)

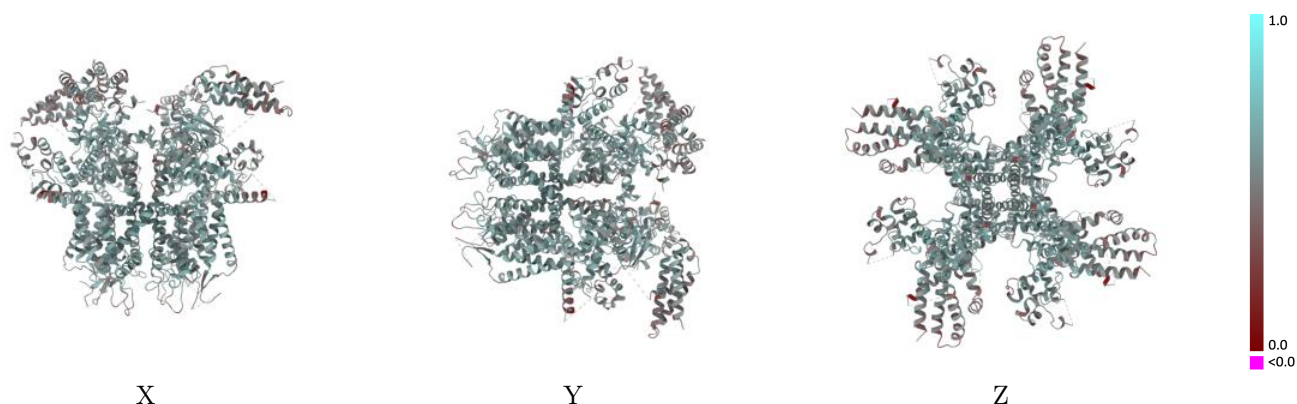
This section contains information regarding the fit between EMDB map EMD-40431 and PDB model 8SEW. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

### 9.1 Map-model overlay [i](#)



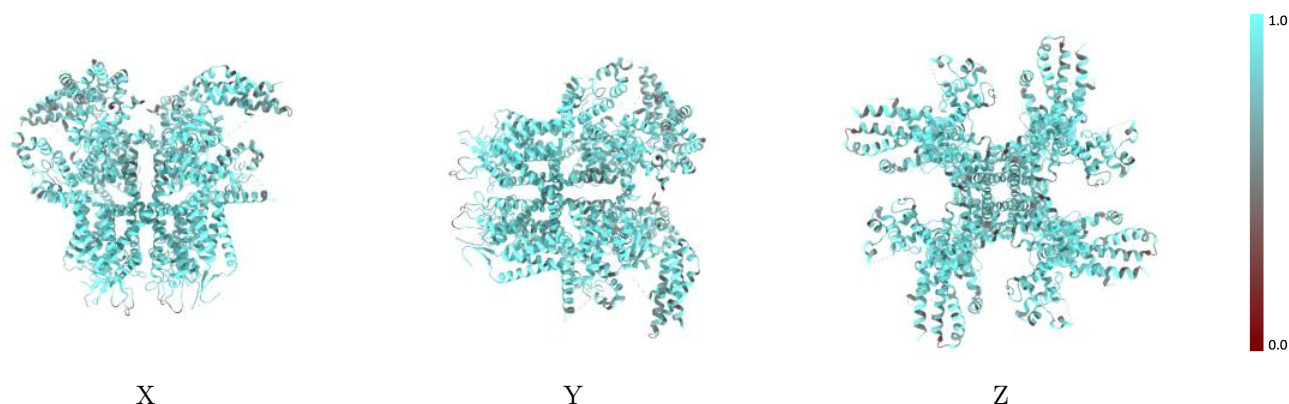
The images above show the 3D surface view of the map at the recommended contour level 0.483 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



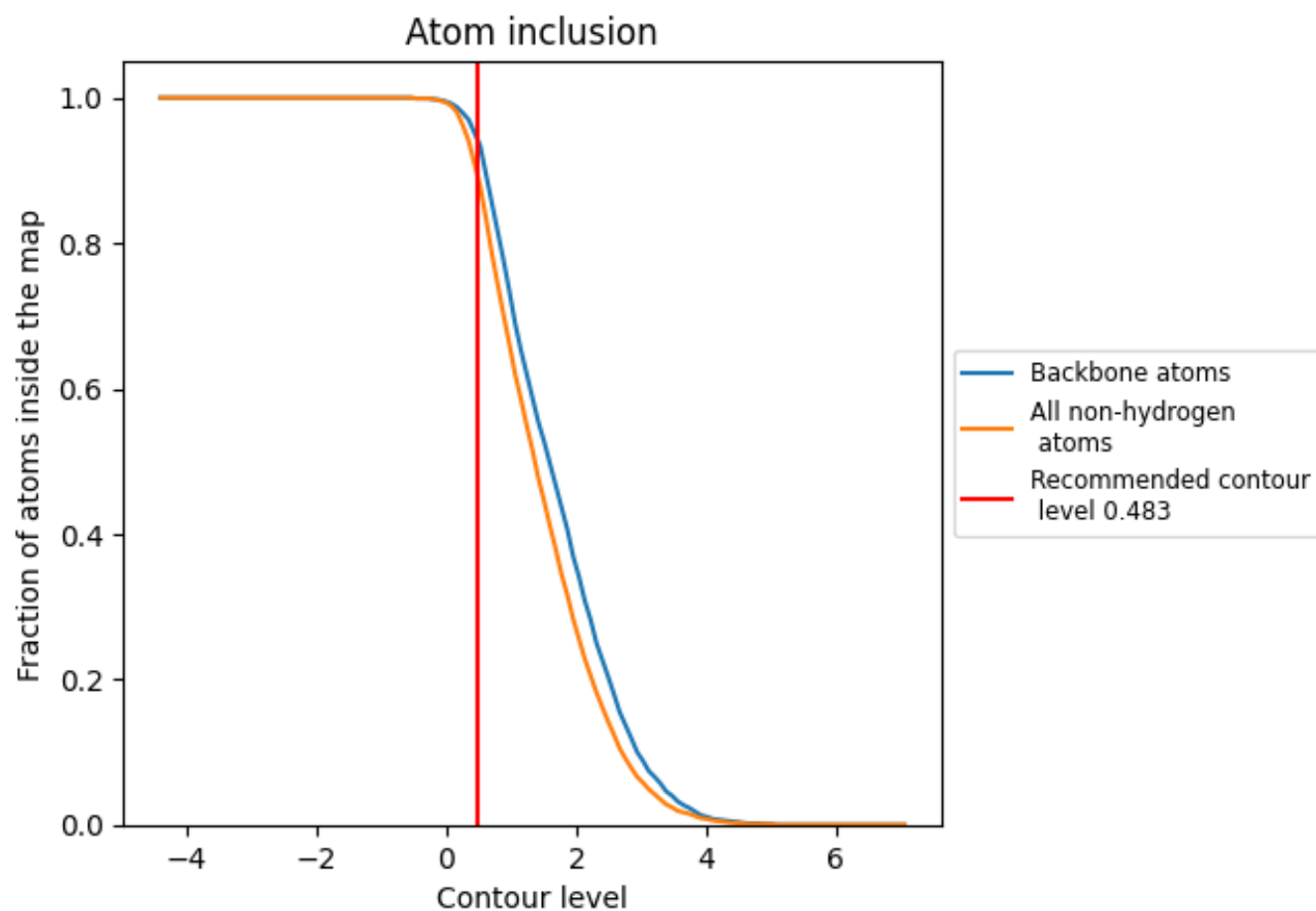
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.483).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.483) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8910	<div></div> 0.5490
A	<div></div> 0.8910	<div></div> 0.5490
B	<div></div> 0.8910	<div></div> 0.5490
C	<div></div> 0.8910	<div></div> 0.5490
D	<div></div> 0.8910	<div></div> 0.5490

